AMENDMENTS TO THE SPECIFICATION

Please replace the title "Molecular Modeling Methods" with the following title:

Method of Modeling Complex Formation Between A Query Ligand and A Target Molecule

Please replace the paragraph beginning at page 27, line 9 with the following amended paragraph:

All software was written at Vertex Pharmaceuticals, Inc. in Python, Perl or C++ unless otherwise noted. Routines that require molecular representation use the Python or C++ interface to the OEChem library (OpenEye Scientific Software, Santa Fe, NM 87507). **X-ray Structures**. FASTA (Pearson, W.R., Lipman, D.J. *PNAS*. 1988, 85 2444-2448) was used to identify X-ray structures in the protein data bank (pdb)(Berman, H.M., et al., *Nucleic Acids Research*. 2000, 28, 235-242) with sequences homologous to the kinase domain of pkaα using a cutoff value of 3. Because a high cutoff value was used, the choice of reference kinase sequence does not affect the results. Only structures containing a ligand that binds to the ATP pocket of the kinase were included in the analysis. For pdb files containing multiple structures of the same kinase domain with different chain names, only the first chain containing the kinase domain was included in the analysis. The X-ray structures were aligned in a common coordinate frame by superimposing backbone atoms (N, CA and C) of residues corresponding to 142 – 149 in thejnk3 hinge region onto the jnk3 reference structure (pdb code 1jnk; Xie, X., et al., Structure. 1998, 6, 983-991) using the McLachlan algorithm (McLachlan, A.D., *Acta Cryst* 1982, A38,871-873) as implemented in the program ProFit (Martin, A.C.R, ~~http://www.bioinf.org.uk/software/profit/~~ ~~http://www.bioinf.org.us/software/profit~~. bioinf.org.us/software/profit.

Please delete the previous abstract at page 53 and add the following new abstract on the following page: